LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042935.D
Acq On : 05 Apr 2021 16:57
Operator : SY/MD
Sample : M1903-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 41749

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Title : SW846 8260

Signal : TIC: VU042935.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.366	3	8	20	rVB	50659	52024	1.08%	0.349%
2	2.639	392	404	416	rBV	30166	58373	1.21%	0.392%
3	2.803	437	455	493	rBV2	14375	67915	1.40%	0.456%
4	4.121	837	865	914	rBV4	111692	670556	13.87%	4.504%
5	4.456	954	969	992	rBV	61280	145583	3.01%	0.978%
6	5.298	1216	1231	1244	rBV	127298	268886	5.56%	1.806%
7	5.382	1244	1257	1278	rVB	206592	417189	8.63%	2.802%
8	5.710	1345	1359	1393	rBV	143070	355170	7.34%	2.386%
9	6.256	1514	1529	1551	rBV	300563	561716	11.62%	3.773%
10	6.546	1601	1619	1654	rBV2	186776	514490	10.64%	3.456%
11	7.906	2027	2042	2053	rBV	468714	801931	16.58%	5.386%
12	7.967	2053	2061	2084	rVB3	33004	72684	1.50%	0.488%
13	8.456	2200	2213	2240	rBV	248085	474096	9.80%	3.184%
14	9.423	2501	2514	2525	rBV	433174	709416	14.67%	4.765%
15	9.491	2525	2535	2568	rVB	650711	1121739	23.20%	7.535%
16	9.925	2659	2670	2686	rVB	38602	63944	1.32%	0.430%
17	10.214	2748	2760	2781	rBV	244408	427214	8.83%	2.870%
18	10.639	2879	2892	2902	rBV	380656	601951	12.45%	4.043%
19	10.693	2902	2909	2924	rVB3	49046	82582	1.71%	0.555%
20	11.237	3062	3078	3085	rBV	107237	174856	3.62%	1.174%
21	11.279	3085	3091	3108	rVV2	90285	161881	3.35%	1.087%
22	11.381	3112	3123	3141	rVB	329663	477100	9.87%	3.205%
23	11.568	3170	3181	3186	rBV5	30192	49411	1.02%	0.332%
24	11.613	3186	3195	3220	rVV	220483	421041	8.71%	2.828%
25	11.729	3222	3231	3249	rVV4	64495	166697	3.45%	1.120%
26	11.819	3249	3259	3275	rVB	502553	783138	16.19%	5.260%
27	12.066	3322	3336	3362	rBV	3017064	4836087	100.00%	32.483%
28	12.182	3365	3372	3403	rVB4	87090	208443	4.31%	1.400%
29	14.198	3989	3999	4013	rBV2	41273	74144	1.53%	0.498%
30	14.291	4019	4028	4048	rVB	37675	67723	1.40%	0.455%

Sum of corrected areas: 14887980

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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
41749

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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Operator : SY/MD
Sample : M1903-06
Misc : 5.0mL/MSVOA_U/WATER
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Instrument : MSVOA_U
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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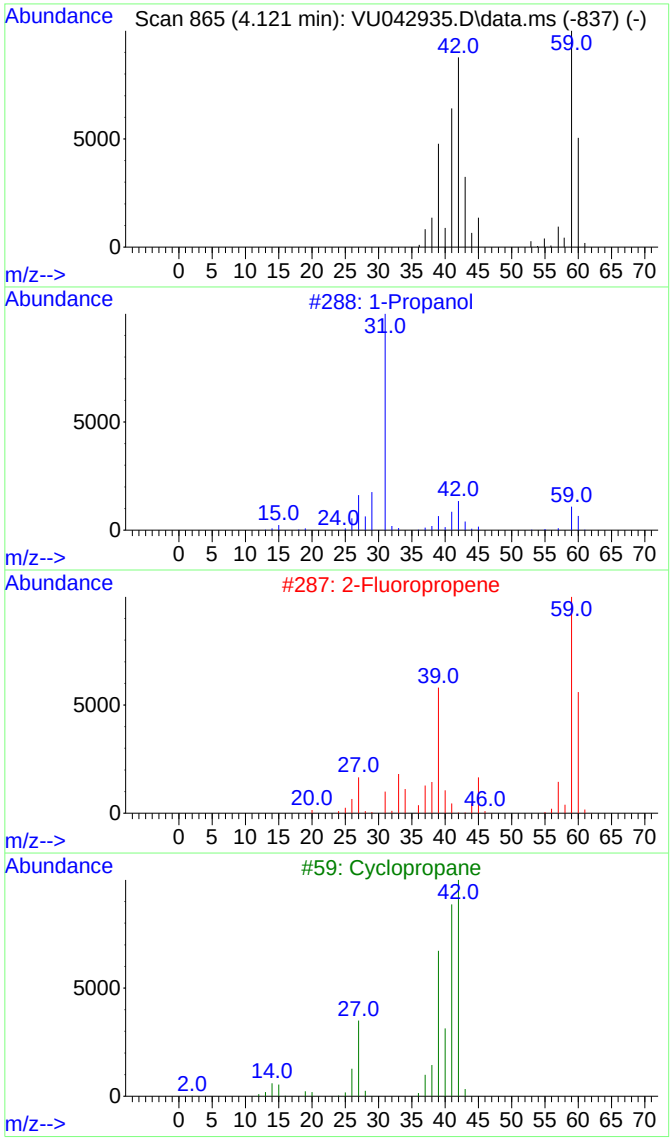
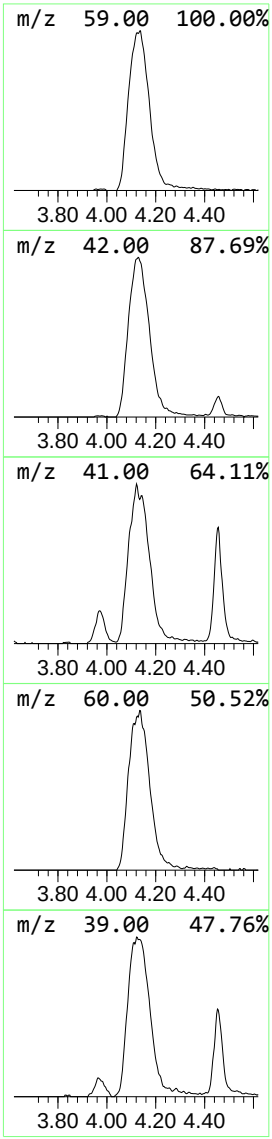
Peak Number 1 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.121	80.37 ug/l	670556	Pentafluorobenzene	5.382

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	64
2	2-Fluoropropene	60	C3H5F	001184-60-7	52
3	Cyclopropane	42	C3H6	000075-19-4	25
4	Allyl fluoride	60	C3H5F	000818-92-8	9
5	2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	9





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Sample : M1903-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 41749

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
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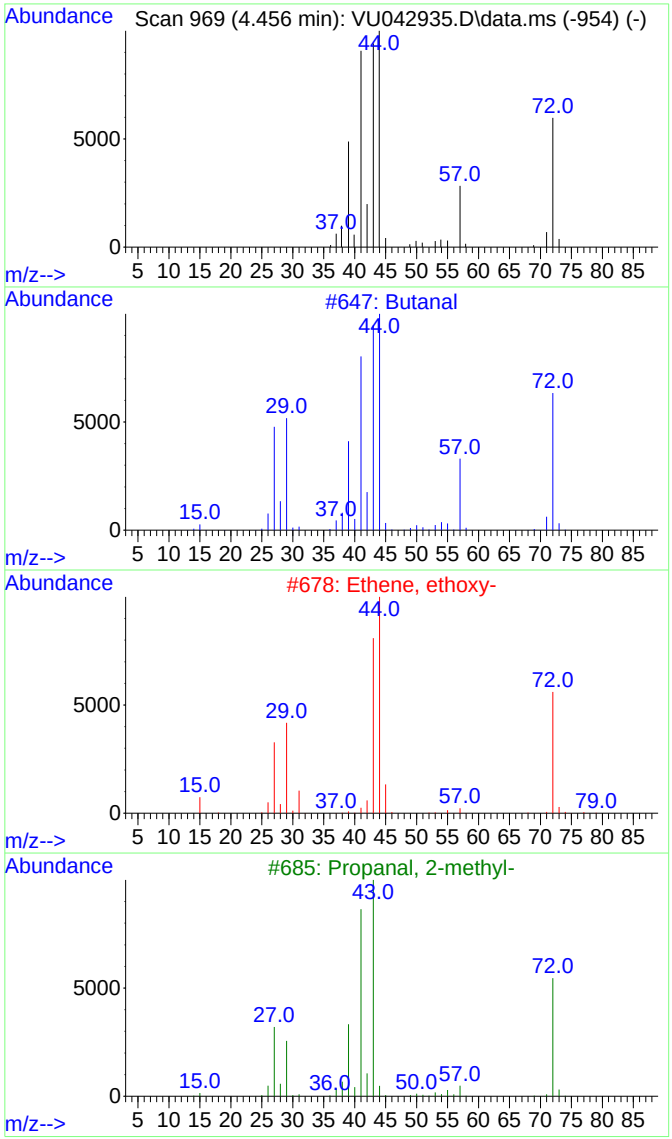
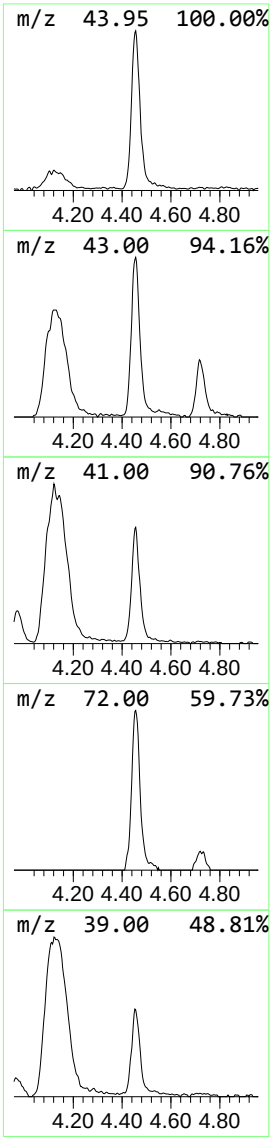
Peak Number 2 Butanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.456	17.45 ug/l	145583	Pentafluorobenzene	5.382

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	47
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38
5	Methacrolein	70	C4H6O	000078-85-3	16





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Operator : SY/MD
Sample : M1903-06
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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 41749

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
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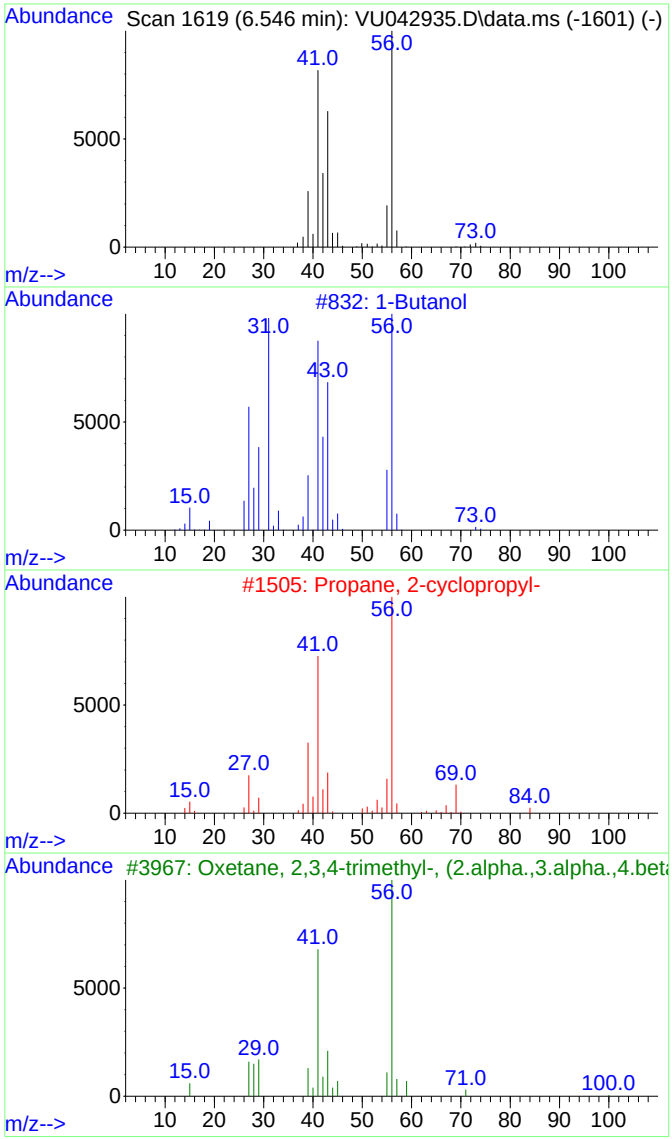
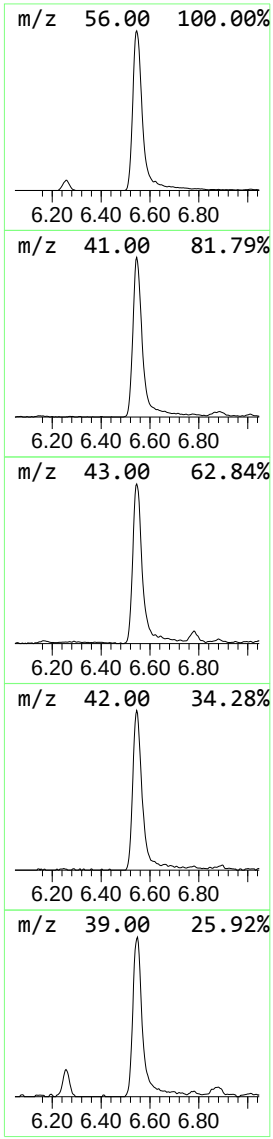
Peak Number 3 1-Butanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.546	45.80 ug/l	514490	1,4-Difluorobenzene	6.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	91
2	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	39
3	Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	9
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	9





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Sample : M1903-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 41749

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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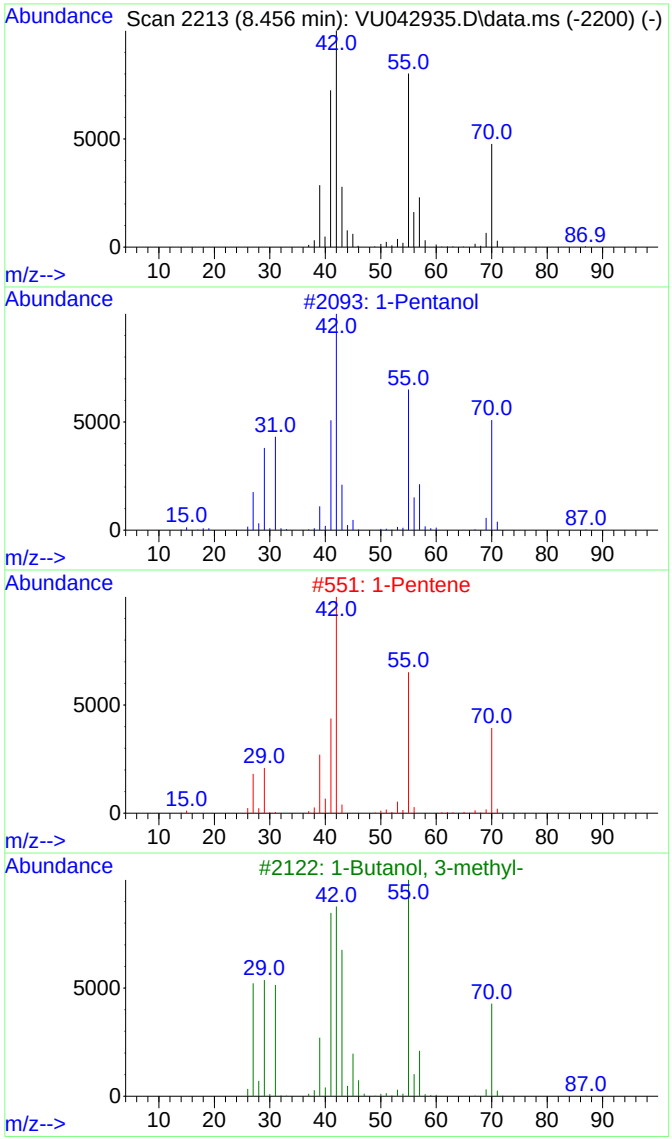
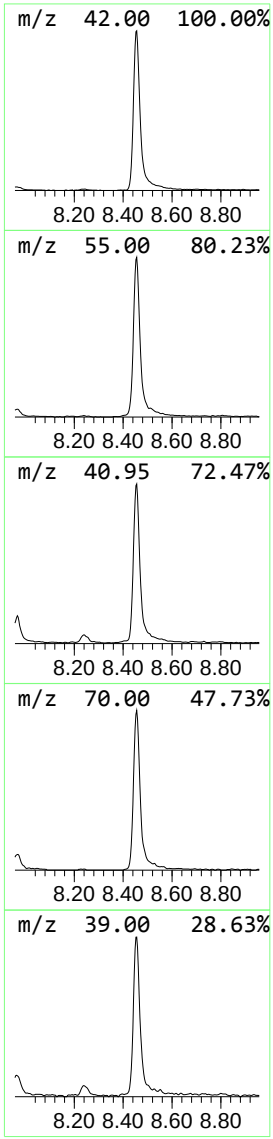
Peak Number 4 1-Pentanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.456	33.41 ug/l	474096	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol	88	C5H12O	000071-41-0	90
2	1-Pentene	70	C5H10	000109-67-1	80
3	1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	64
4	Carbonochloridic acid, pentyl ester	150	C6H11ClO2	000638-41-5	43
5	Formic acid, pentyl ester	116	C6H12O2	000638-49-3	40





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Sample : M1903-06
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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 41749

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
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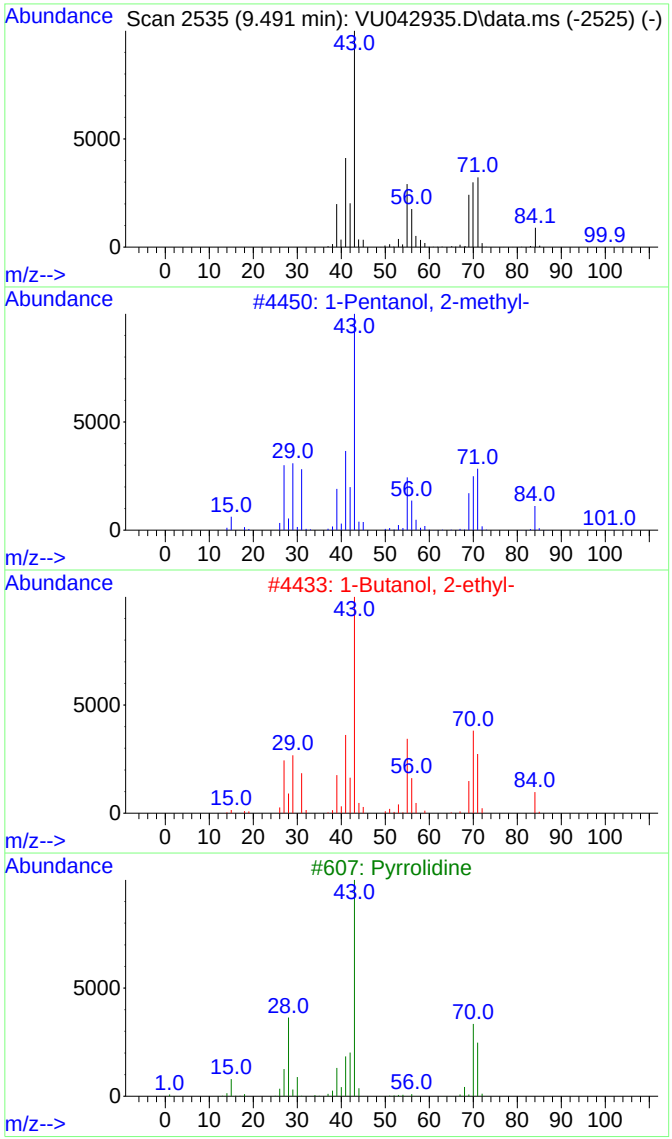
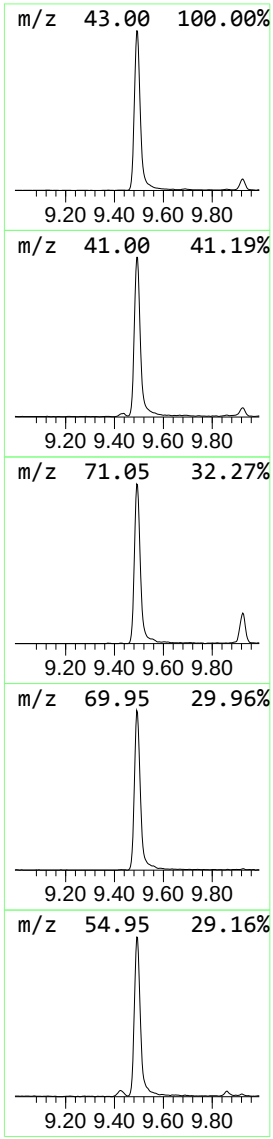
****
Peak Number 5 1-Pentanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.491	79.06 ug/l	1121740	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	90
2	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	83
3	Pyrrolidine	71	C4H9N	000123-75-1	59
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	47
5	Butane, 1-bromo-3-methyl-	150	C5H11Br	000107-82-4	45





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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 41749

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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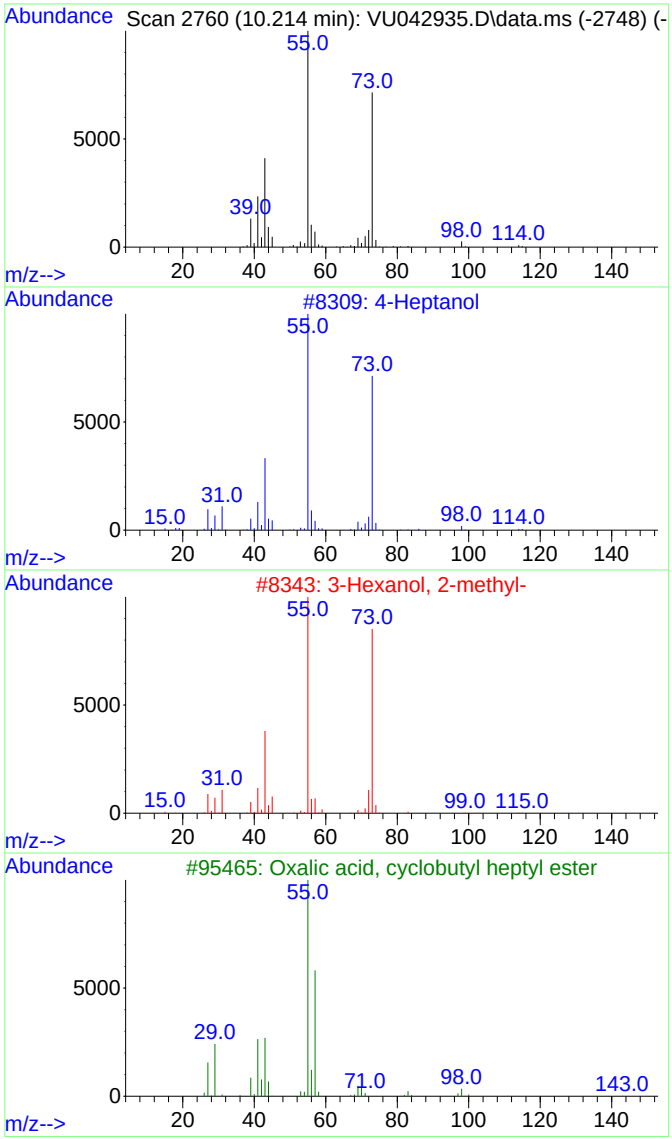
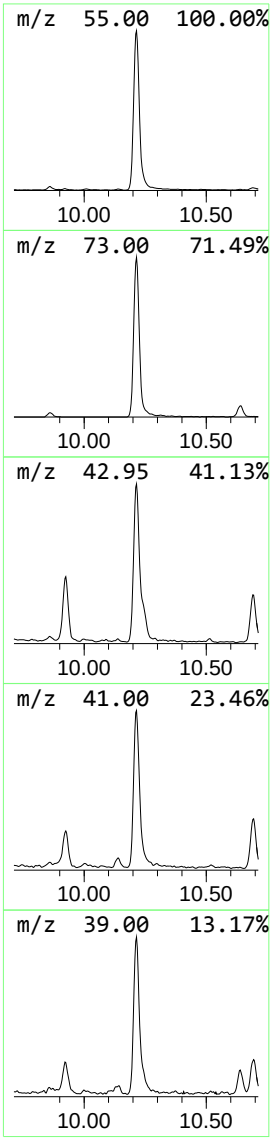
Peak Number 6 4-Heptanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.214	30.11 ug/l	427214	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol	116	C7H16O	000589-55-9	83
2	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	45
3	Oxalic acid, cyclobutyl heptyl e...	242	C13H22O4	1000309-69-8	40
4	Isobutylamine	73	C4H11N	000078-81-9	37
5	Oxalic acid, cyclobutyl hexyl ester	228	C12H20O4	1000309-69-7	35





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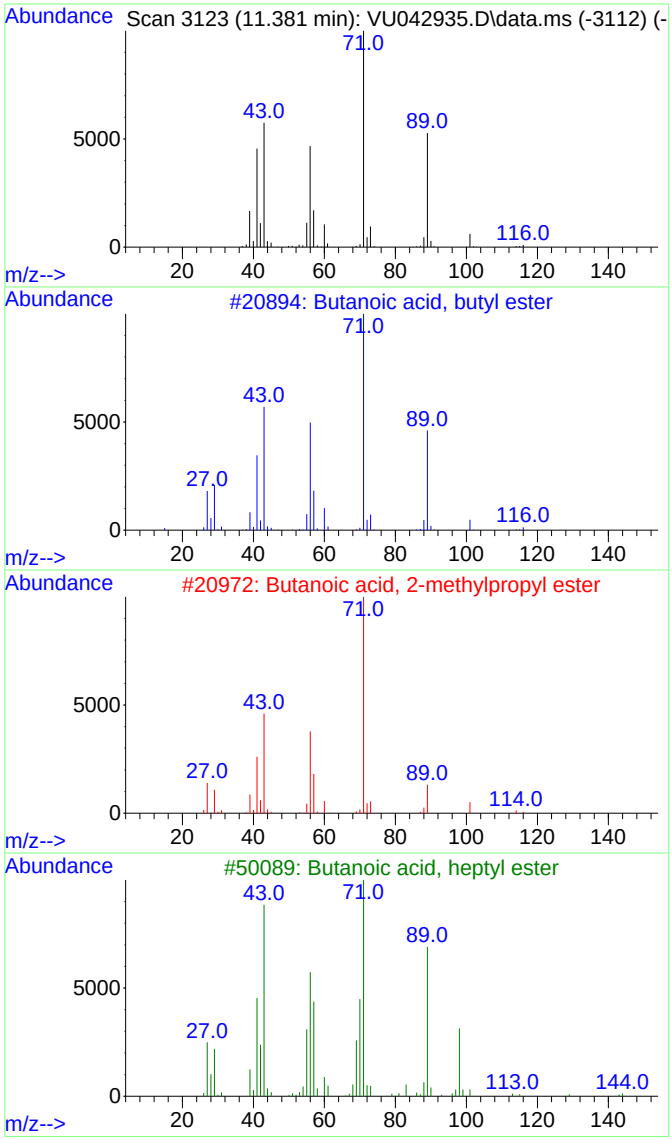
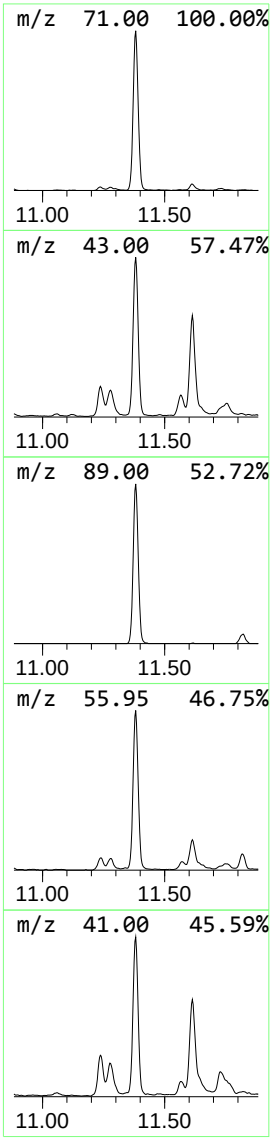
Peak Number 7 Butanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.382	30.46 ug/l	477100	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
3	Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	72
4	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	64
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59





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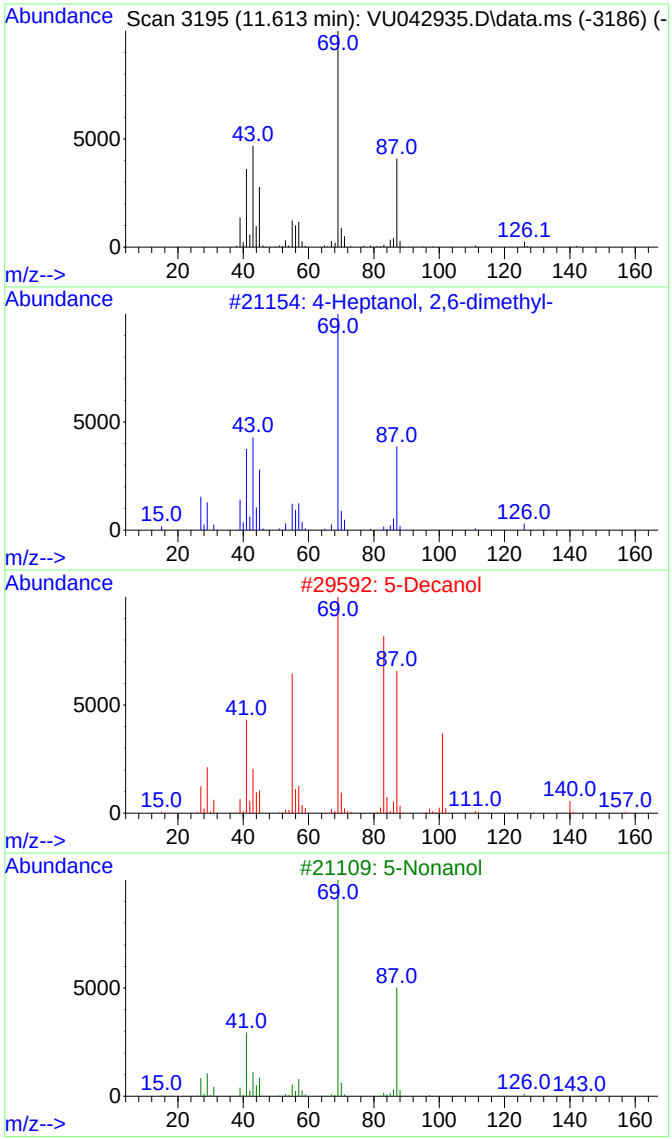
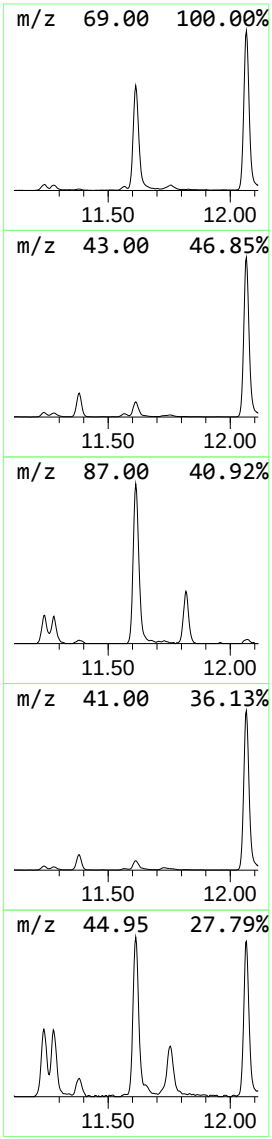
Peak Number 8 4-Heptanol, 2,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.613	26.88 ug/l	421041	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	90
2	5-Decanol	158	C10H22O	005205-34-5	72
3	5-Nonanol	144	C9H20O	000623-93-8	72
4	1-Octyn-4-ol	126	C8H14O	052517-92-7	64
5	4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	64





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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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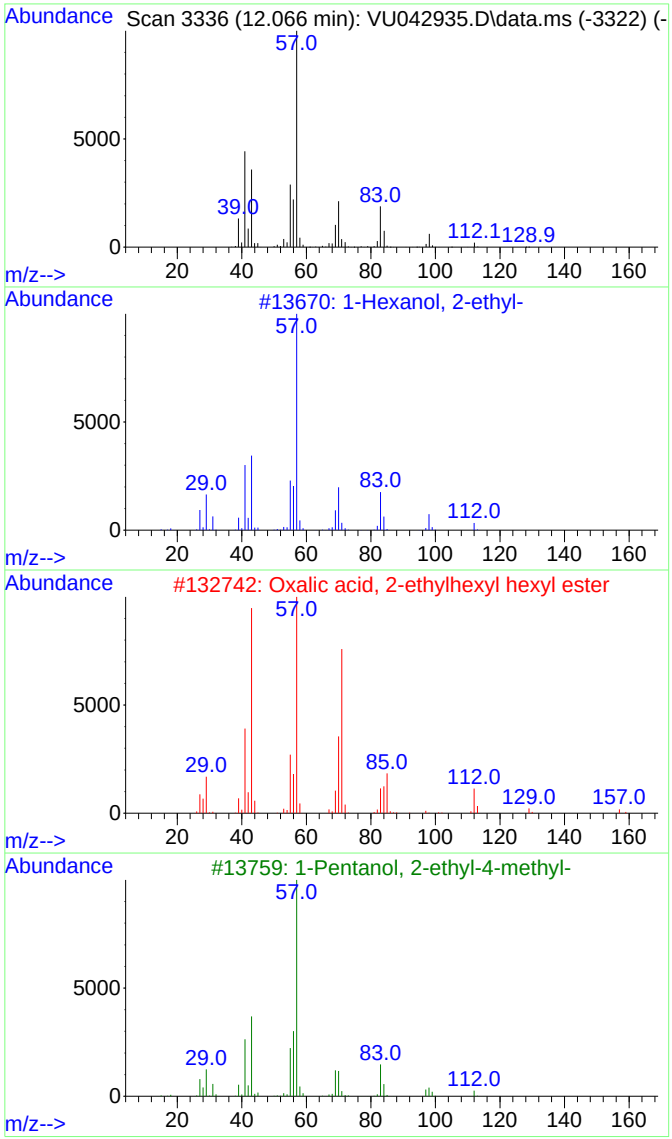
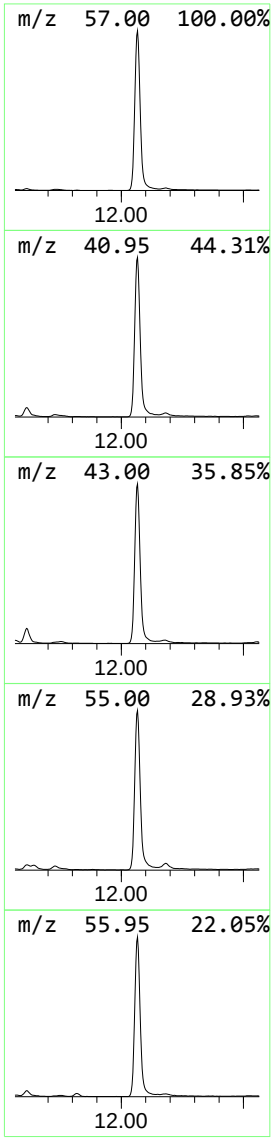
Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.066	308.76 ug/l	4836090	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Oxalic acid, 2-ethylhexyl hexyl ...	286	C16H30O4	1000309-38-9	59
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50





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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
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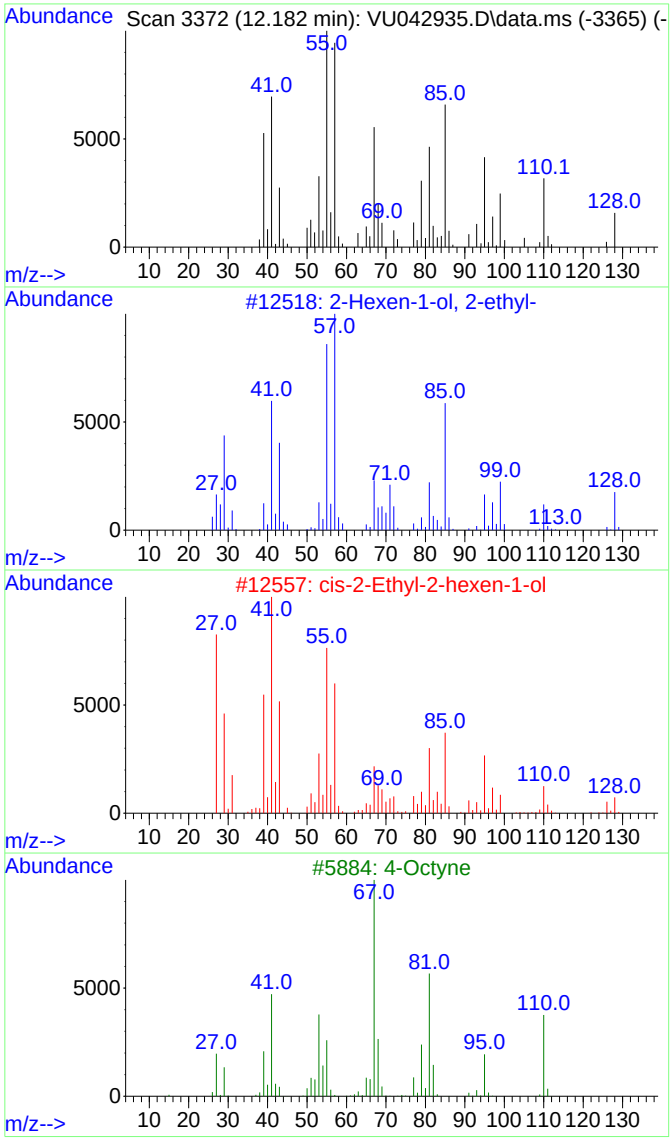
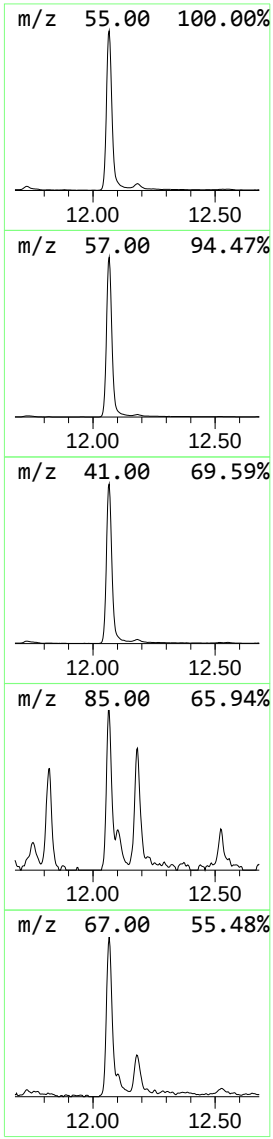
Peak Number 10 2-Hexen-1-ol, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.182	13.31 ug/l	208443	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexen-1-ol, 2-ethyl-	128	C8H16O	050639-00-4	60
2	cis-2-Ethyl-2-hexen-1-ol	128	C8H16O	1000139-52-4	46
3	4-Octyne	110	C8H14	001942-45-6	42
4	Cyclohexene, 1,6-dimethyl-	110	C8H14	001759-64-4	35
5	4-Methyl-1,4-heptadiene	110	C8H14	013857-55-1	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
Data File : VU042935.D
Acq On : 05 Apr 2021 16:57
Operator : SY/MD
Sample : M1903-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 41749

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1-Propanol	4.121	80.4	ug/l	670556	1	5.382	417189	50.0
Butanal	4.456	17.4	ug/l	145583	1	5.382	417189	50.0
1-Butanol	6.546	45.8	ug/l	514490	2	6.256	561716	50.0
1-Pentanol	8.456	33.4	ug/l	474096	3	9.423	709416	50.0
1-Pentanol, 2-m...	9.491	79.1	ug/l	1121740	3	9.423	709416	50.0
4-Heptanol	10.214	30.1	ug/l	427214	3	9.423	709416	50.0
Butanoic acid, ...	11.382	30.5	ug/l	477100	4	11.819	783138	50.0
4-Heptanol, 2,6...	11.613	26.9	ug/l	421041	4	11.819	783138	50.0
1-Hexanol, 2-et...	12.066	308.8	ug/l	4836090	4	11.819	783138	50.0
2-Hexen-1-ol, 2...	12.182	13.3	ug/l	208443	4	11.819	783138	50.0